## A Quick Look at THz Attenuation Mechanisms and Propagation

Two types of attenuation, both more common than in lower RF bands:

(1) **Absorption**
- Conversion of electromagnetic radiation into heat
(a) Conduction current (Joule) heating: $P_{diss} = \overline{\mathbf{J} \cdot \mathbf{E}}$
(e.g., losses in undepleted semiconductors)
(overbar denotes time average)
(b) Polarization current heating $P_{diss} = \overline{(d\mathbf{P}/dt) \cdot \mathbf{E}}$
(e.g., polar liquids, such as water in a microwave oven)

(2) **Scattering**
(a) Non-resonant internal scattering from inhomogeneous dielectrics
(e.g., composite materials such as RT-Duroid)
(b) Resonant scattering from particles of dimension $\sim\lambda$ (e.g., raindrops)
(c) Mixture of specular scattering from smooth surfaces and
diffuse scattering from rough surfaces (in infrared, more surfaces
tend to be diffuse; in RF bands more surfaces tend to be specular)

# Radiative Transfer
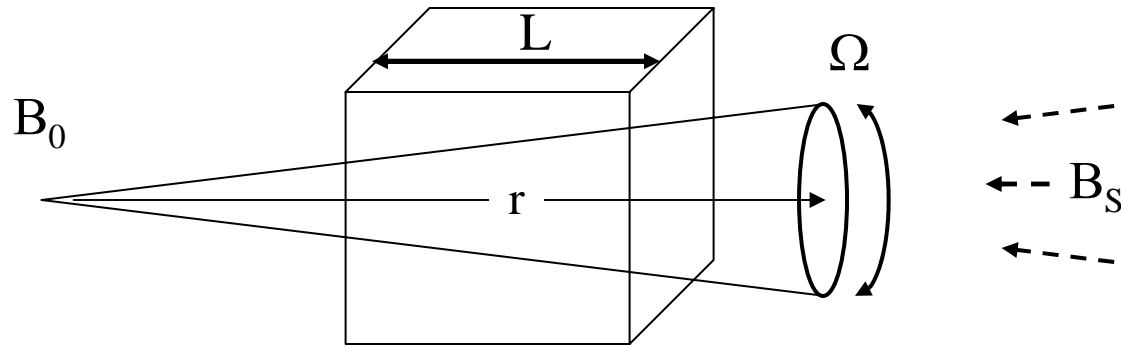


$$\frac{dB}{dr} + \alpha B = \frac{\rho J}{4\pi} \qquad \text{1D Radiative Transport Equation}$$

$\alpha \rightarrow$ attenuation constant ; $\quad \rho \rightarrow$ density ; $\quad$ J $\rightarrow$ emission coefficient

$$B(r) = B_S \exp(-\tau) + (\rho J/4\pi\alpha)[1 - \exp(-\tau)] \qquad \tau = \int_0^L \alpha(r)dr$$

Homogeneous Solution $\qquad$ Particular Solution $\qquad$ "Optical Depth"

Special Cases: (1) $j = 0 \Rightarrow B = B_S \exp(-\tau)$ Beer-Lambert Law

(2) $B = \text{uniform} \Rightarrow dB = 0 \Rightarrow B = (\rho J/4\pi\alpha)$ Kirchoff's Law

Good Introductory Reference: J.D. Kraus, "Radio Astronomy" (McGraw-Hill, New York, 1966).

## Beer-Lambert Law

Describes attenuation effects for many THz point sensors (active and passive), and for remote active systems. Especially useful when intervening material is a linear, isotropic, and homogeneous (LIH) dielectric, or an array of independent scatterers:

$$T \equiv \frac{I_t}{I_i} = \exp(-\alpha_A \cdot z)$$

$T \rightarrow$ transmission, $\alpha_A \rightarrow$ attenuation coefficient

$I_i \rightarrow$ incident intensity, $I_t \rightarrow$ transmitted intensity

For absorption, $\alpha_A = \alpha_{ABS}$, the absorption coefficient
(a characteristic of the material, and generally a function of frequency)

For scattering $\alpha_A = \rho \, \sigma_S$, $\rho$ being the density and $\sigma_S$ the scattering cross section

# Atmospheric Attenuation Simulation

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## Simulation Tool:

- Windows®-based atmospheric propagation tool called PcLnWin (Ontar, Corp.)
- FASCODE radiative transfer engine developed by U.S. Air Force Geophysics Lab in 1970s.
- HITRAN96 database (> 1 million molecular lines) developed by molecular chemists and maintained by U.S. Air Force (Hanscom AFB)

## Atmospheric Conditions

- Seven "standard" molecules: $H_2O$, $CO_2$, $O_3$, $N_2O$, $CO$, $CH_4$, $O_2$

- 1976 U.S. standard atmospheric model @ sea level
    - Temperature = 288 K, Pressure = 1 atm, Humidity = 46%

<div style="border:1px solid red; color:red">

**Between 300 GHz and 2.0 THz, water vapor dominates the attenuation by way of molecular dipole transitions**

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## Stick Diagram of Atmospheric Molecular Lines
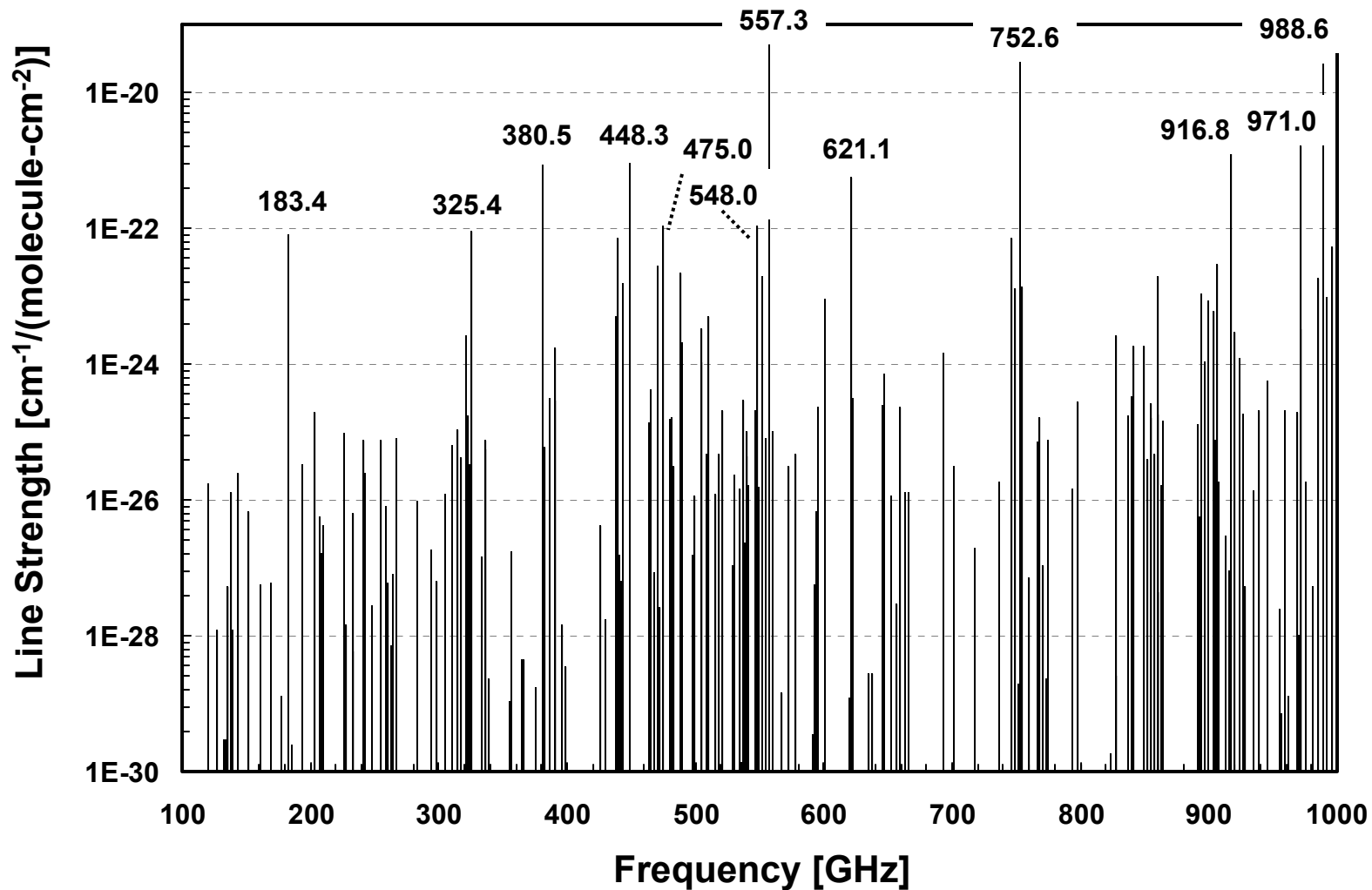
# Why is Water Vapor Absorption So Strong and So Complicated ?

- **For all polar molecules in the vapor state, THz transitions can occur between angular momentum eigenstates of the entire molecule if the energy difference between eigenstates = h$\nu$, and if the change in angular momentum along the axis of photon propagation = h/2$\pi$**

- **For symmetric rotors (e.g., carbom monoxide CO, hydrogen chloride HCl, etc.), two of the moments (along two orthogonal axes) are identical and the third is trivially small, so that**

$$\overset{\longleftarrow \ R \ \longrightarrow}{(+)\!\!-\!\!\!-\!\!\!-\!\!\!-\!\!(-)} \qquad \mathbf{I = \mu R^2} \qquad \textbf{Ignoring spin, } \mathbf{U_X = \dfrac{L^2}{2I_X}} \qquad L^2 = \hbar^2 l(l+1)$$
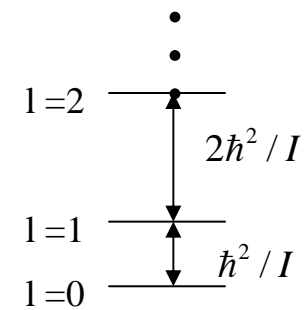
$I_X \rightarrow$ **moment of inertia for rotation about a given axis, x**
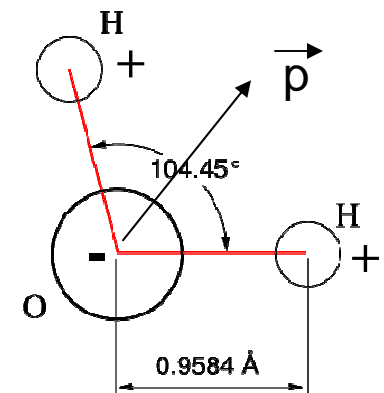$L \rightarrow$ **orbital angular momentum eigenvalue**

- **Photon absorption or emission can occur of $\Delta$l = 1, for which**

$$\Delta U = \frac{\hbar^2}{2I_X}[(l+1)(l+2) - l(l+1)] = \frac{\hbar^2}{I}(l+1) = \hbar\omega$$

**This creates a "ladder" of photon frequencies as shown to the right**

- **Although highly polar, water is asymmetric rotor meaning that no two moments of inertia are equal. This follows from its non-colinear alignment between the three atoms**

- **Any of these purely rotational transitions will be easily observed if $\omega\tau$ >> 1 where $\tau$ is the momentum relaxation time (or dephasing time)**
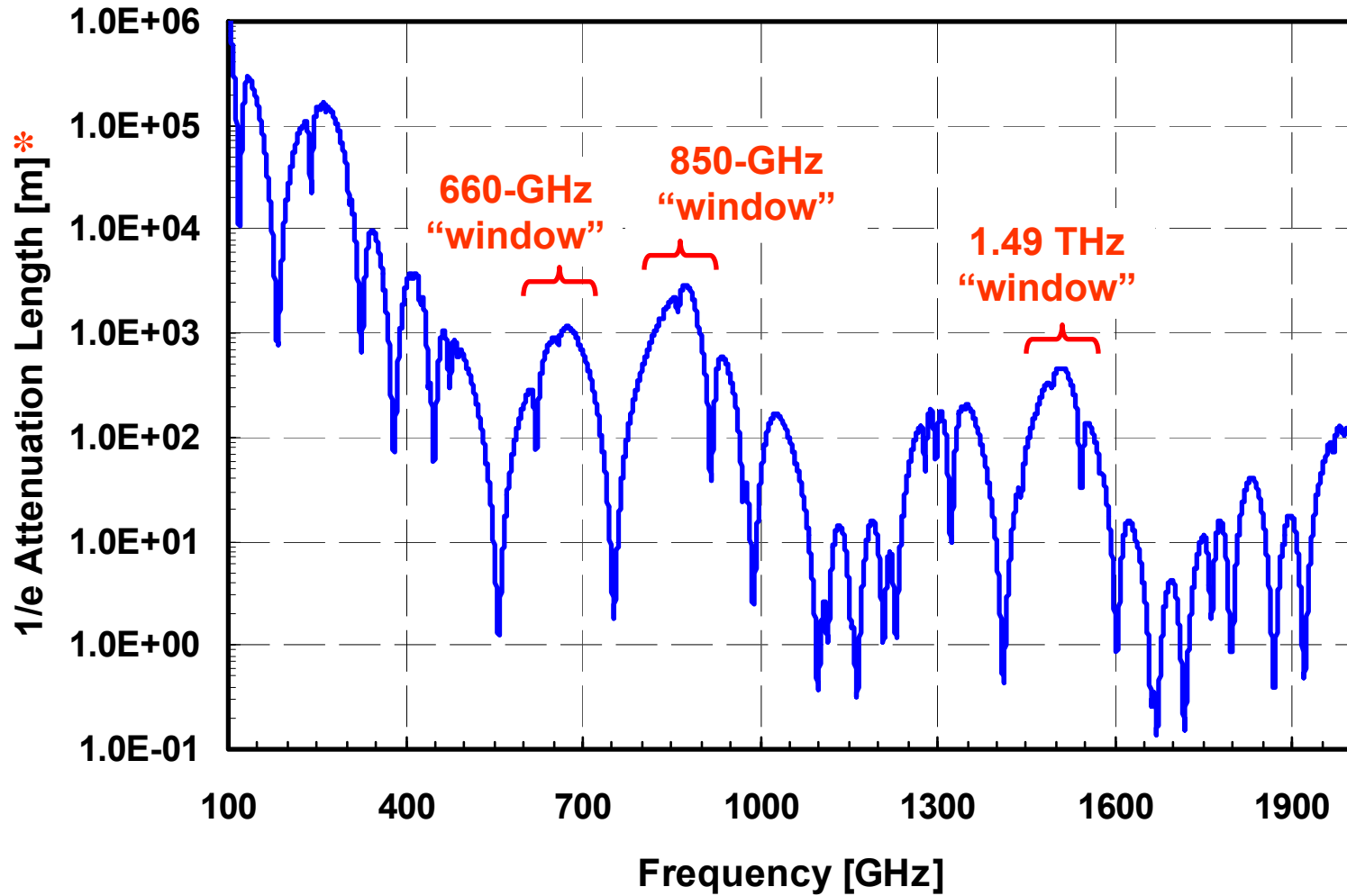
- **Generally, $\tau$ > 100 ps or more under STP conditions, so THz transitions are obvious**

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## Atmospheric Simulation, Propagation "Windows"
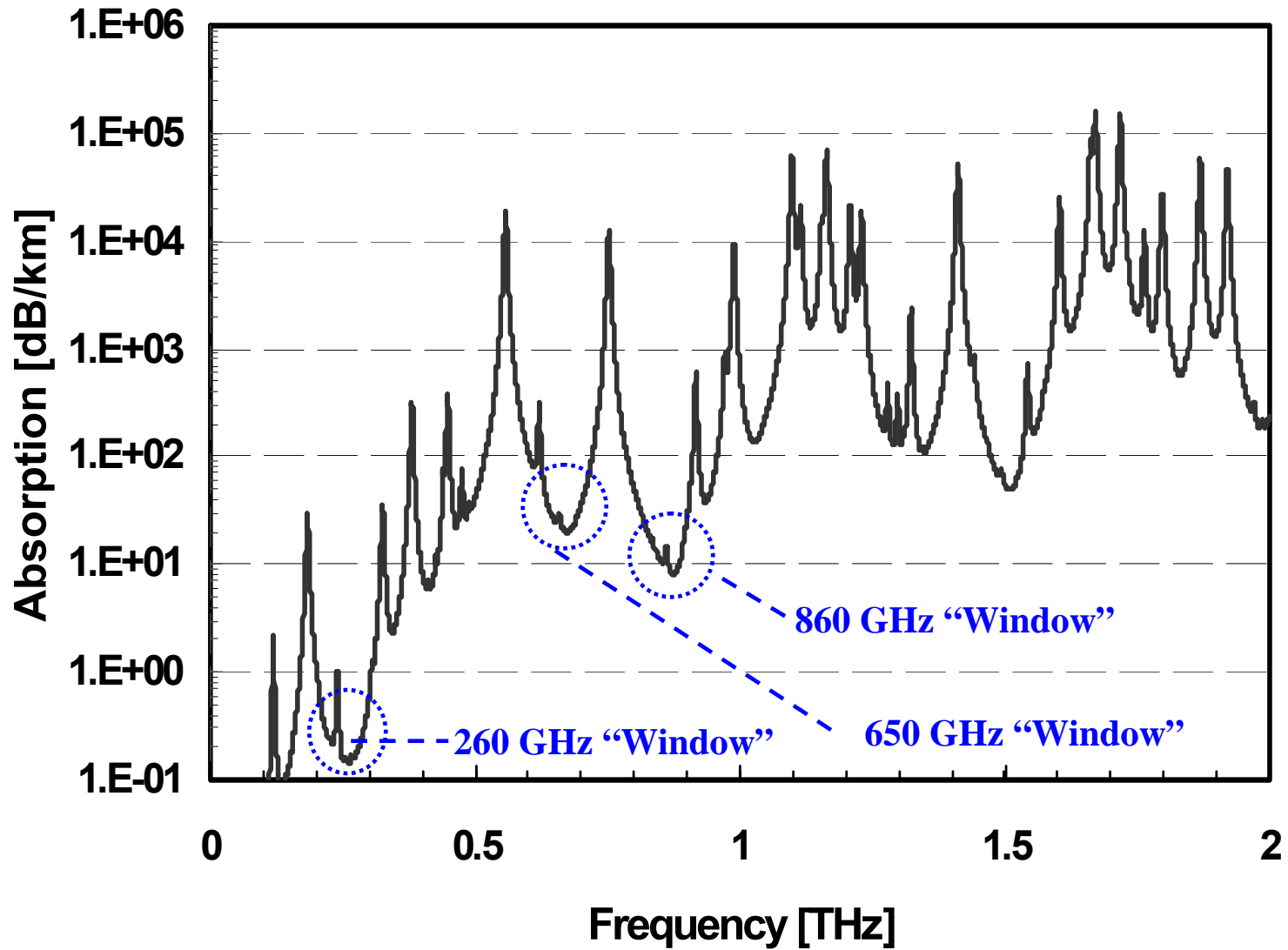
# Equivalent Attenuation Length



**\* Since Lambert-Beer law of transmission, T = exp(-$\alpha$z) applies the 1/e attenuation length is a "natural" metric**

# Ten Strongest Water Vapor Lines in THz Region
## (the big "whoppers")

| Freq [THz] | Peak Attenuation [dB/m] |
|---|---|
| 0.558 | 18.4 |
| 0.758 | 12.7 |
| 0.989 | 9.4 |
| 1.098 | 61.6 |
| 1.164 | 71.6 |
| 1.412 | 52.9 |
| 1.671 | 163.6 |
| 1.718 | 150.0 |
| 1.869 | 59.9 |
| 1.920 | 46.3 |

## Absorption Models for Liquids and Solids

(1) Drude model of conductors :

$$\varepsilon = \varepsilon_{back} - j\frac{\sigma}{\omega} \qquad \sigma = \frac{\sigma_0}{1 - j\omega\tau} \quad \begin{cases} \tau \rightarrow \text{momentum relaxation time} \\ \sim 10 \text{ fs in common metals } @300 \text{ K} \\ > 100 \text{ fs in semiconductors } @300 \text{ K} \end{cases}$$

(2) Debye model of polar liquids (single component):

<u>Single Debye</u>                          <u>Double Debye</u>

$$\varepsilon = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{1 + j(v/v_1)} \qquad \varepsilon = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_1}{1 + j(v/v_1)} + \frac{\varepsilon_1 - \varepsilon_\infty}{1 + j(v/v_2)}$$
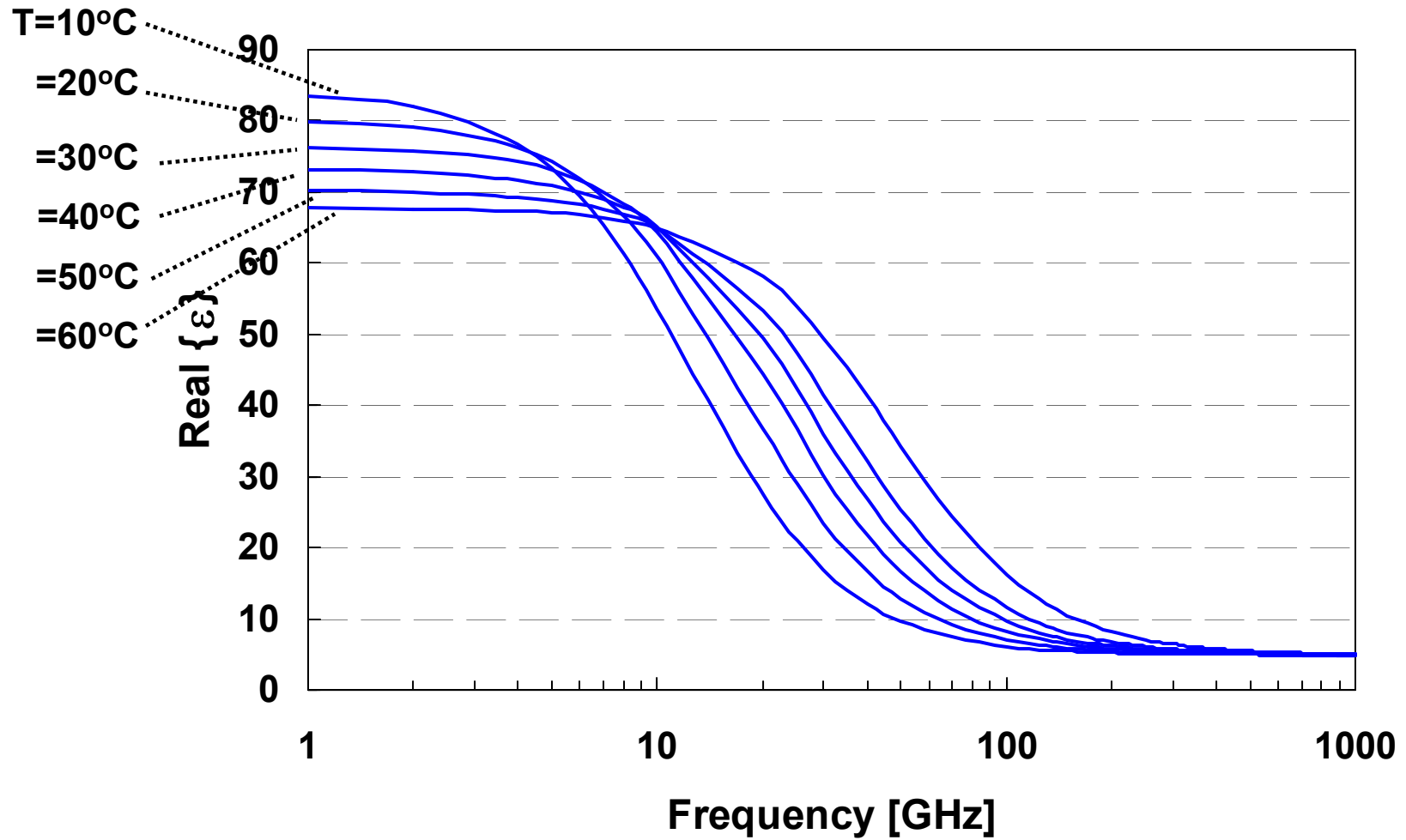
e.g., for pure water at 300 K, single Debye relaxation frequency $v_1 = 17.5$ GHz, and the dielectric constants $\varepsilon_0$ and $\varepsilon_\infty$ are 79.7 and 5.26, respectively

(3) Independent of absorption model, Maxwell's eqns predict:

$$\alpha = 2\omega\left\{\frac{\mu\varepsilon'}{2}\left[\sqrt{1 + (\varepsilon''/\varepsilon')^2} - 1\right]\right\}^{1/2} \qquad \text{where} \quad \varepsilon \equiv \varepsilon' + j\varepsilon''$$
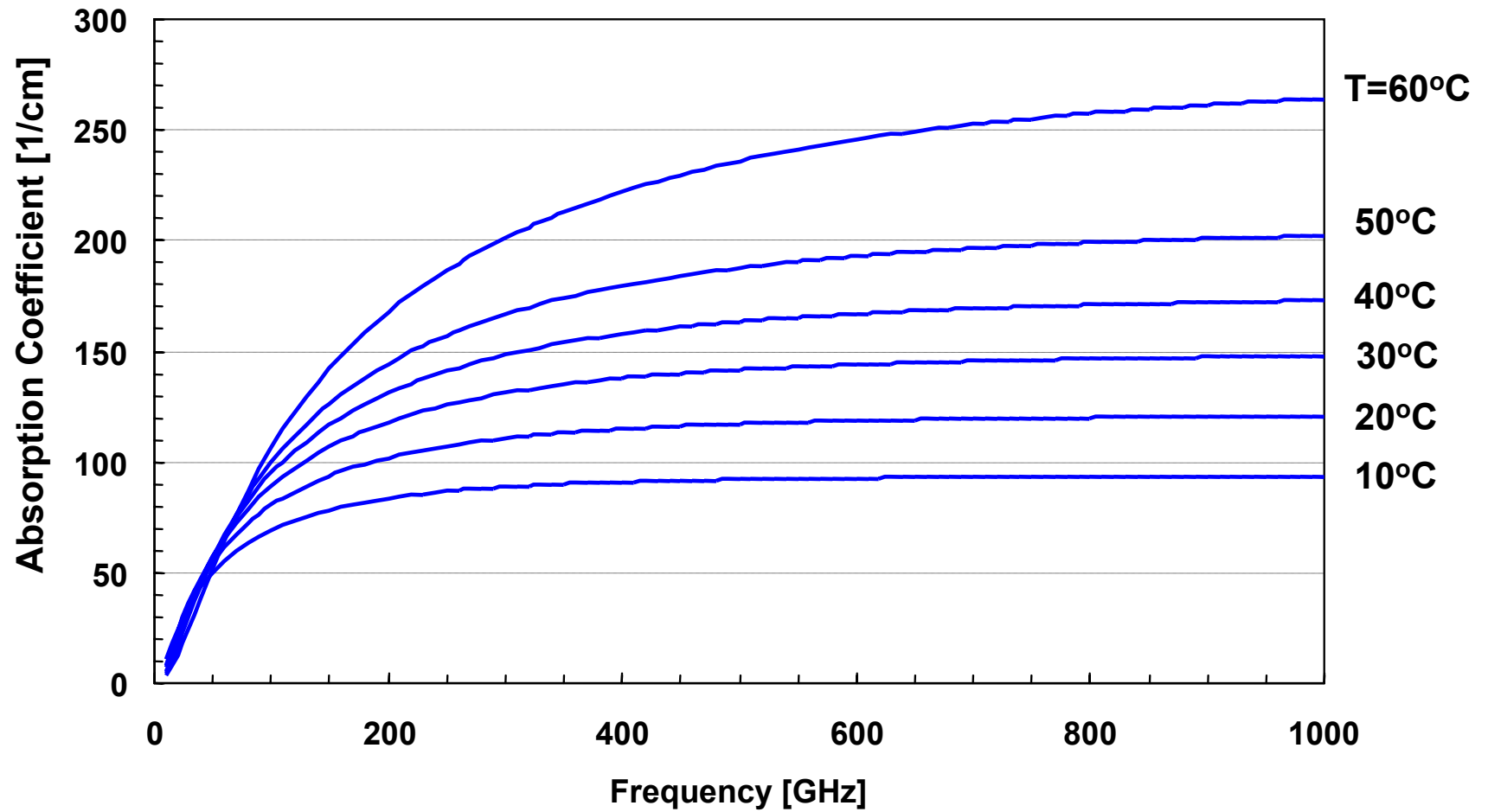
# Single-Debye Model for Liquid Water

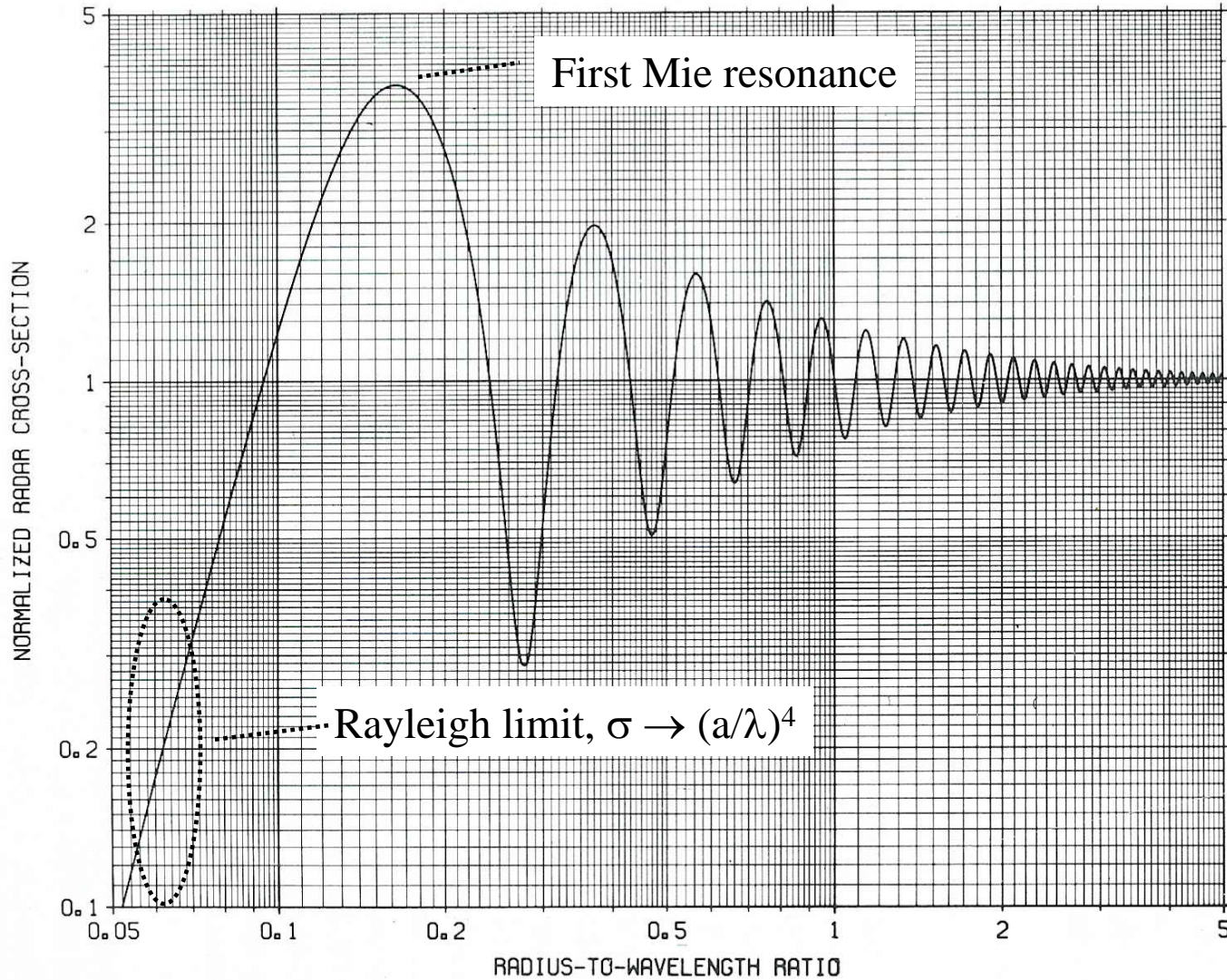$(\varepsilon_0 = 78.2, \varepsilon_\infty = 4.9, \tau = 8.1 \text{ ps, all at } 25^{\circ}\text{C})$

# Single-Debye Model for Liquid Water (cont)

$(\varepsilon_0 = 78.2, \varepsilon_\infty = 4.9, \tau = 8.1 \text{ ps}, \text{ all at } 25^oC)$

## Scattering from a Conducting Sphere



First Mie resonance

Rayleigh limit, $\sigma \rightarrow (a/\lambda)^4$

NORMALIZED RADAR CROSS-SECTION

RADIUS-TO-WAVELENGTH RATIO

**[L.V. Blake, "Radar Range Performance Analysis," (Artech House, Norwoood, MA, 1986), Fig. 3-1].**

## Resonant Scattering

The maximum is $\sigma \approx 3.65 \, \pi a^2$ at a $= 0.163 \, \lambda$. This is called resonant (Mie) scattering and is caused by consructive interference of surface currents flowing around the sphere. Same effect occurs in ellipsoids and arbitary-shaped solids… just not as strong as in spheres
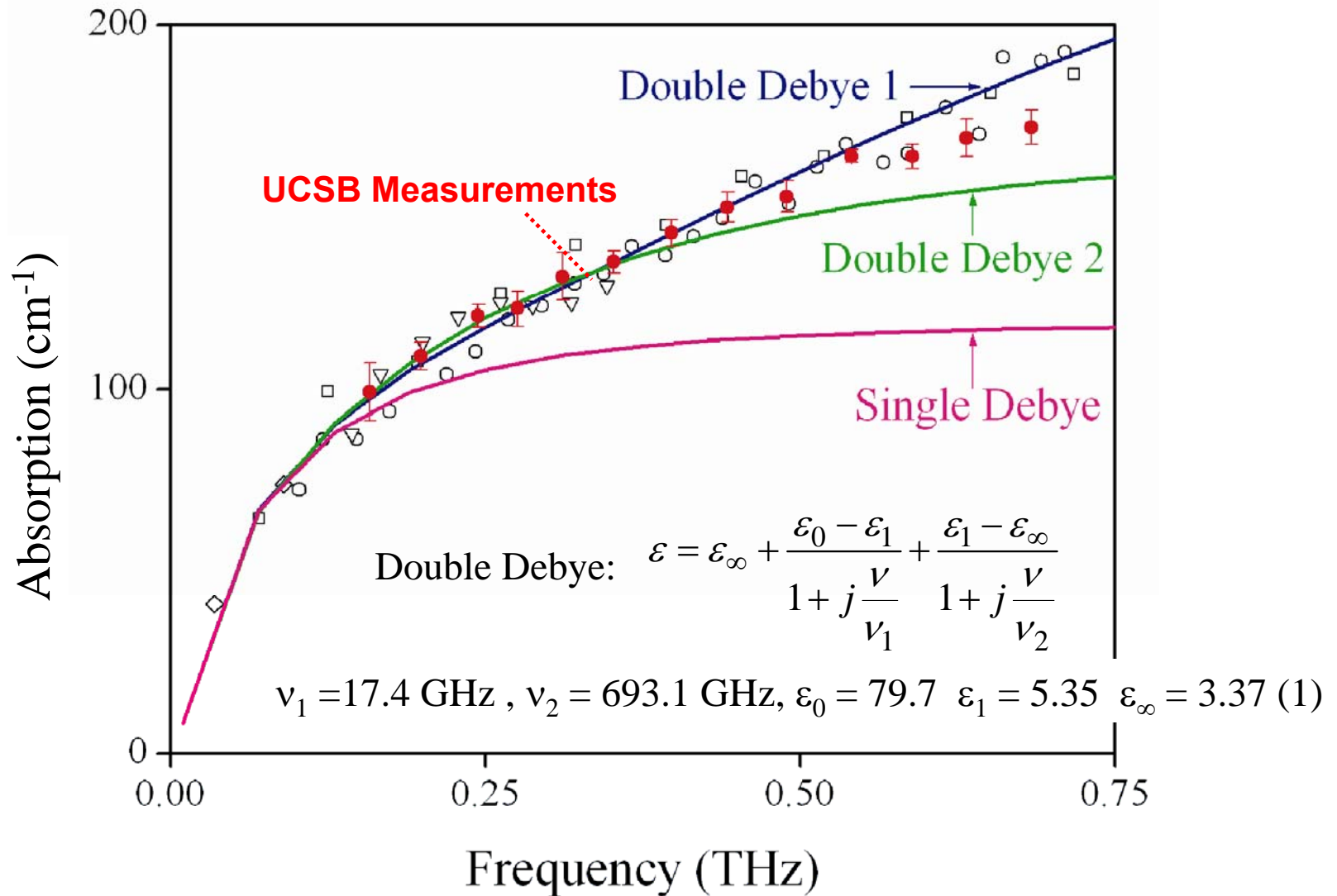
**J (surface current)**

**J**
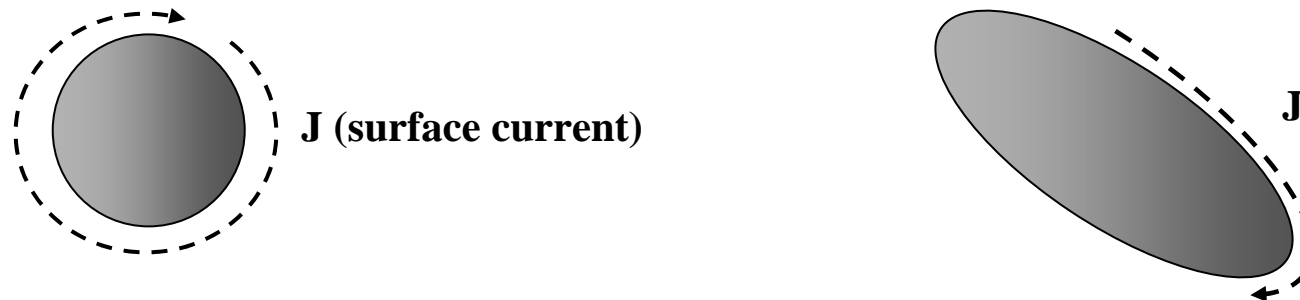
Intuitive estimate of surface resonance assuming surface current velocity of c:
$$2\pi = \omega t = \omega(2\pi a/c) \quad \Rightarrow \quad a = \lambda/2\pi = 0.159 \, \lambda$$

Example: at 1.0 THz ($\lambda = 333 \, \mu m$), resonant Mie scattering occurs for a particle diameter of 106 $\mu m$
• Many materials (e.g., powders such as sugar; composites such as RT-Duroid) have inhomogeneity on the 100 micron scale $\Rightarrow$ strong THz scattering

## Pure Liquid Water at THz Frequencies

**UCSB Measurements**

Double Debye 1 →

Double Debye 2

Single Debye

Absorption (cm$^{-1}$)

Double Debye: $\varepsilon = \varepsilon_\infty + \dfrac{\varepsilon_0 - \varepsilon_1}{1 + j\dfrac{v}{v_1}} + \dfrac{\varepsilon_1 - \varepsilon_\infty}{1 + j\dfrac{v}{v_2}}$

$v_1 = 17.4$ GHz , $v_2 = 693.1$ GHz, $\varepsilon_0 = 79.7$  $\varepsilon_1 = 5.35$  $\varepsilon_\infty = 3.37$ (1)

Frequency (THz)

**(1) H. J. Liebe, G. A. Hufford, and T. Manabe, Int. J. Infr. Millim. Waves, 12, 659 (1991).**

# Salt Water
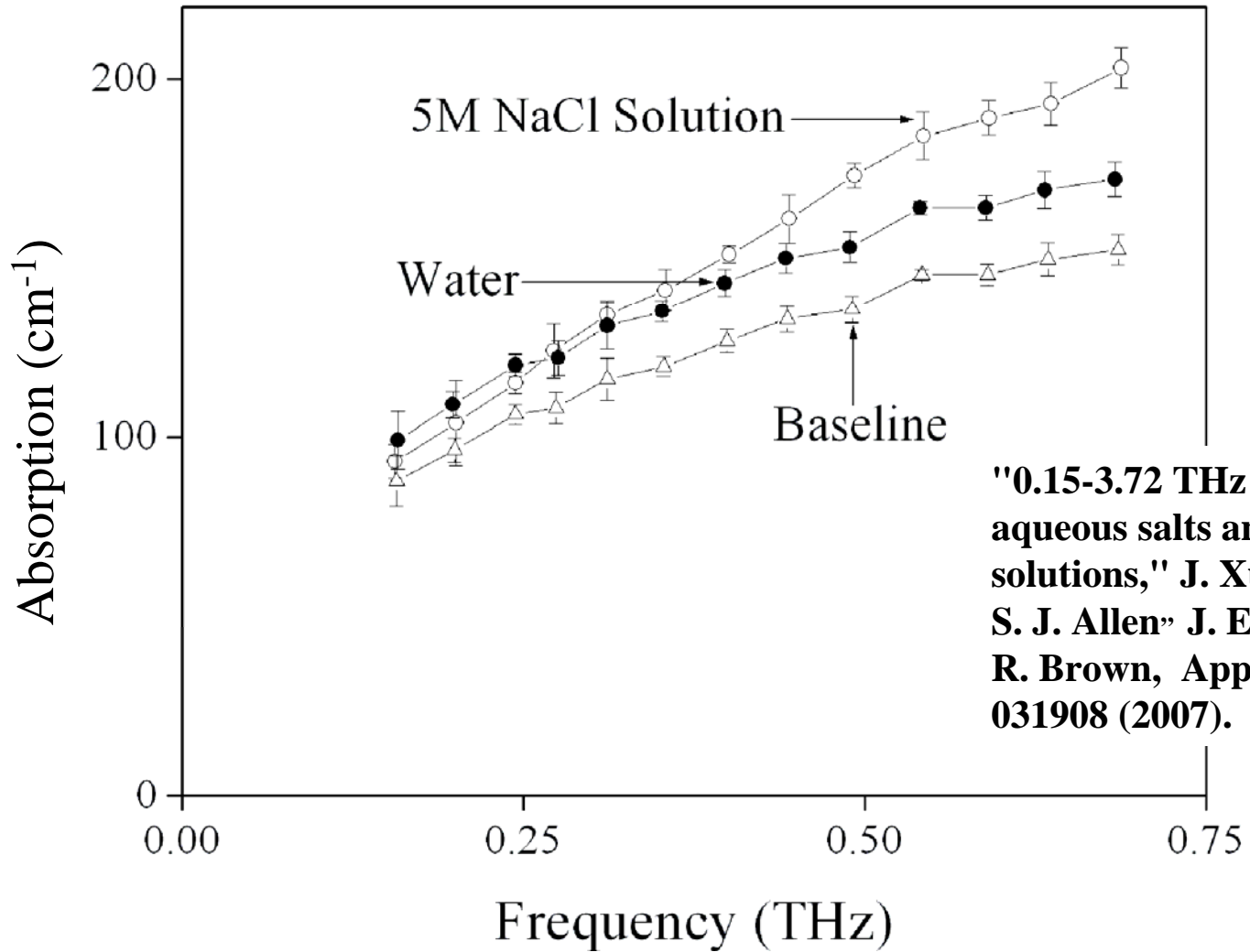


**"0.15-3.72 THz absorption of aqueous salts and saline solutions," J. Xu, K. W. Plaxco, S. J. Allen" J. E. Bjarnason, E. R. Brown, Appl. Phys. Lett, 90, 031908 (2007).**
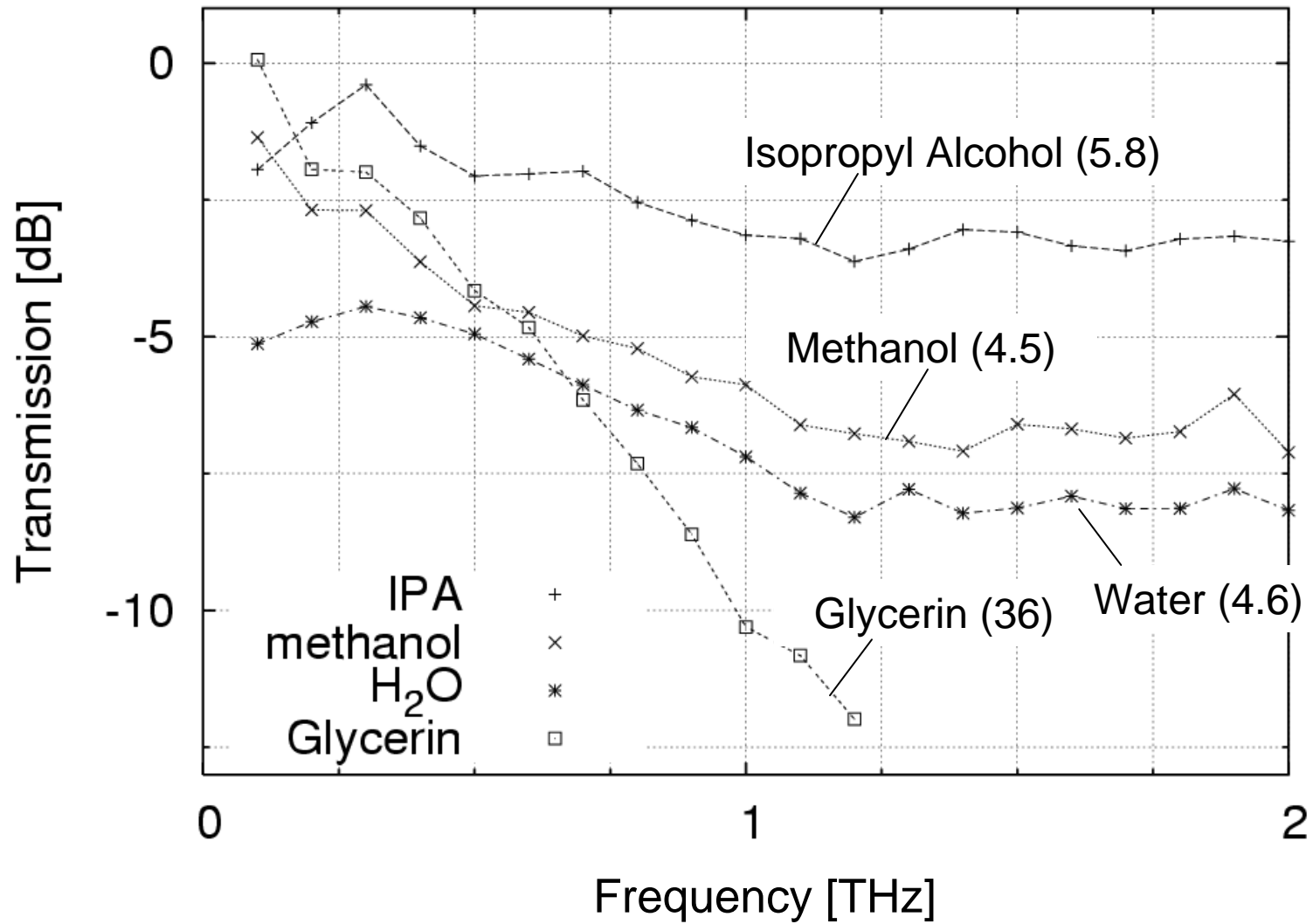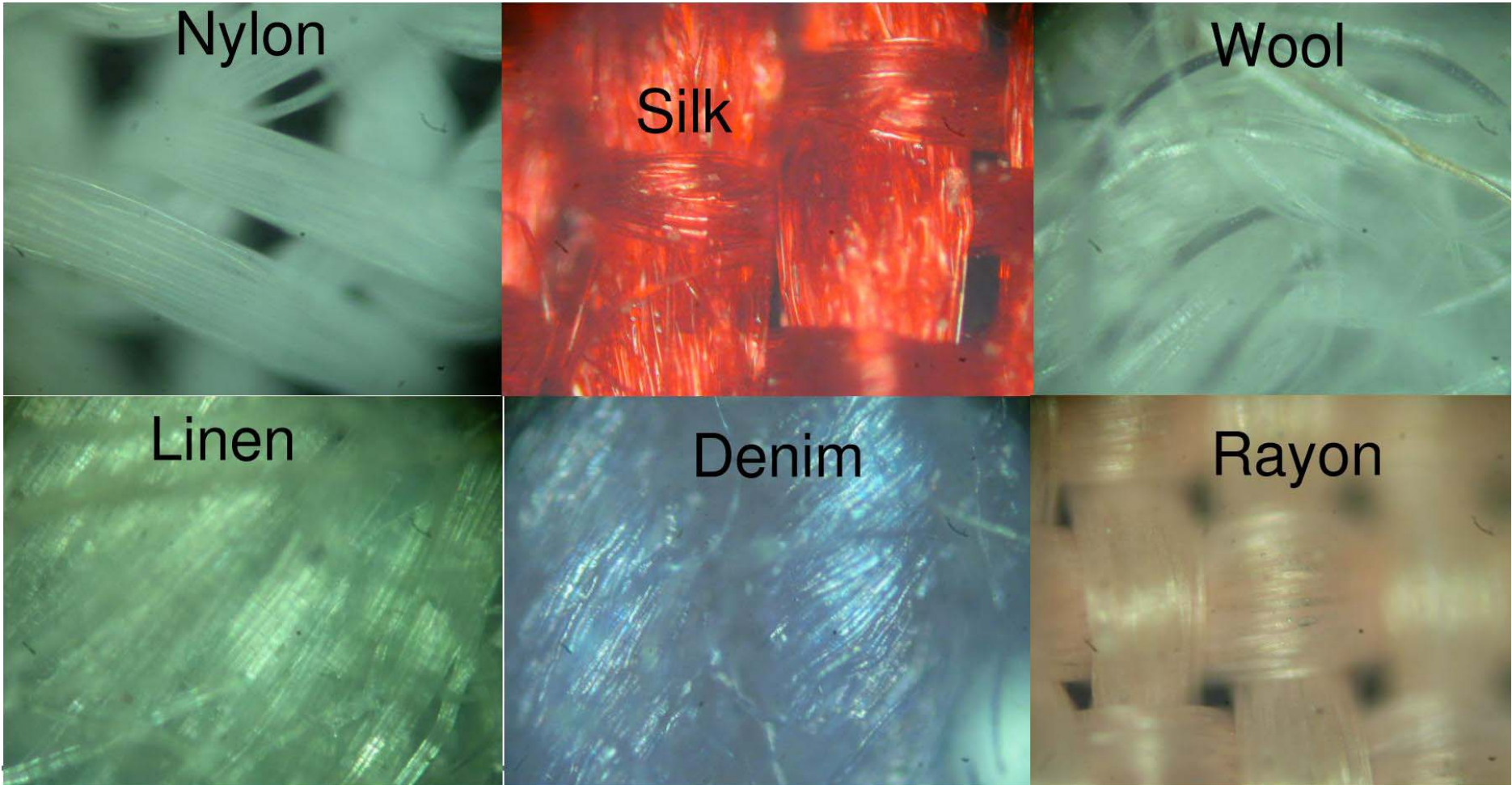
# Disagreement about Salt Water
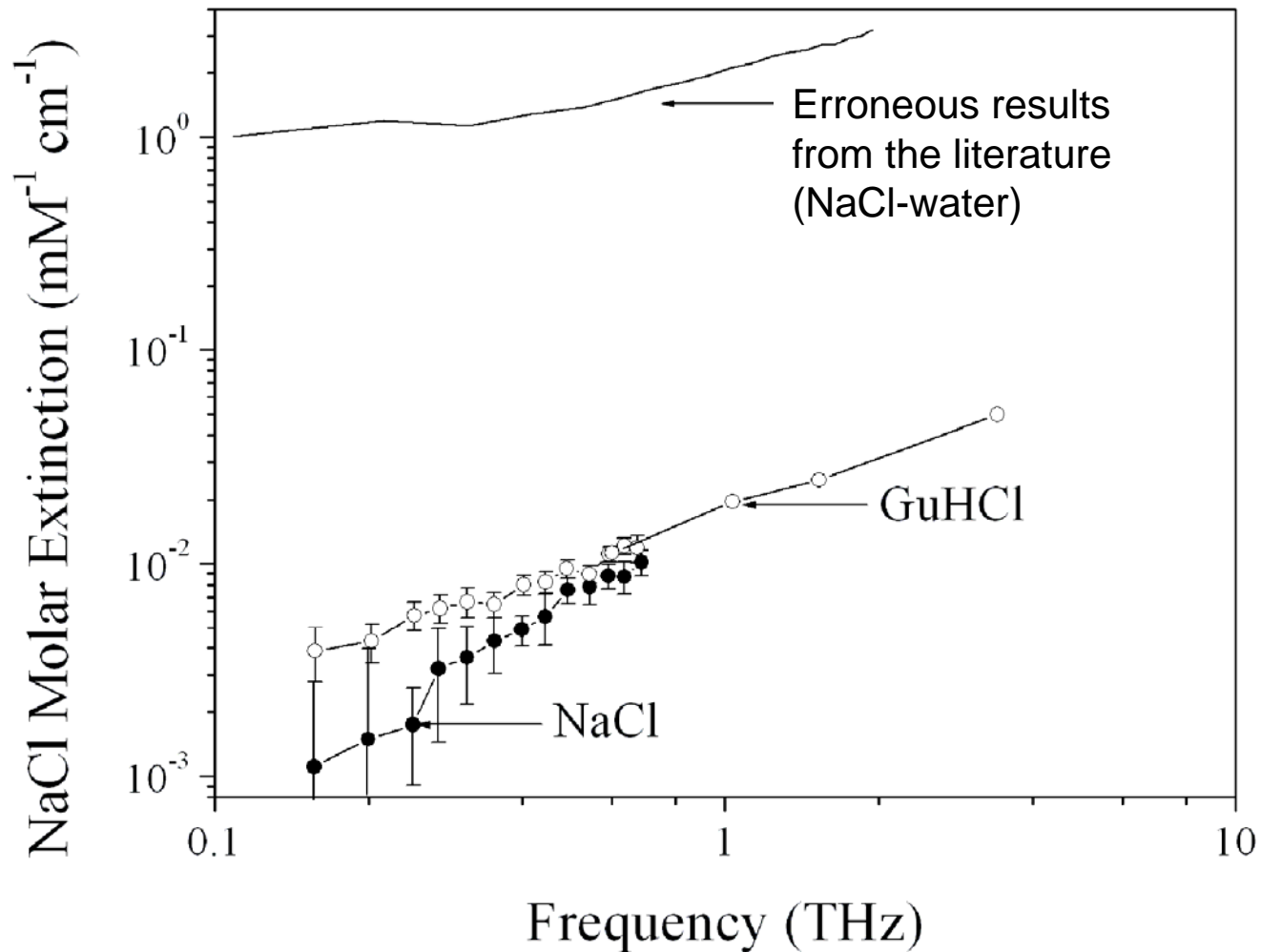


"0.15-3.72 THz absorption of aqueous salts and saline solutions," J. Xu, K. W. Plaxco, S. J. Allen, J. E. Bjarnason, E. R. Brown,  Appl. Phys. Lett, 90, 031908 (2007).

## Other Liquids of Varying Polarity
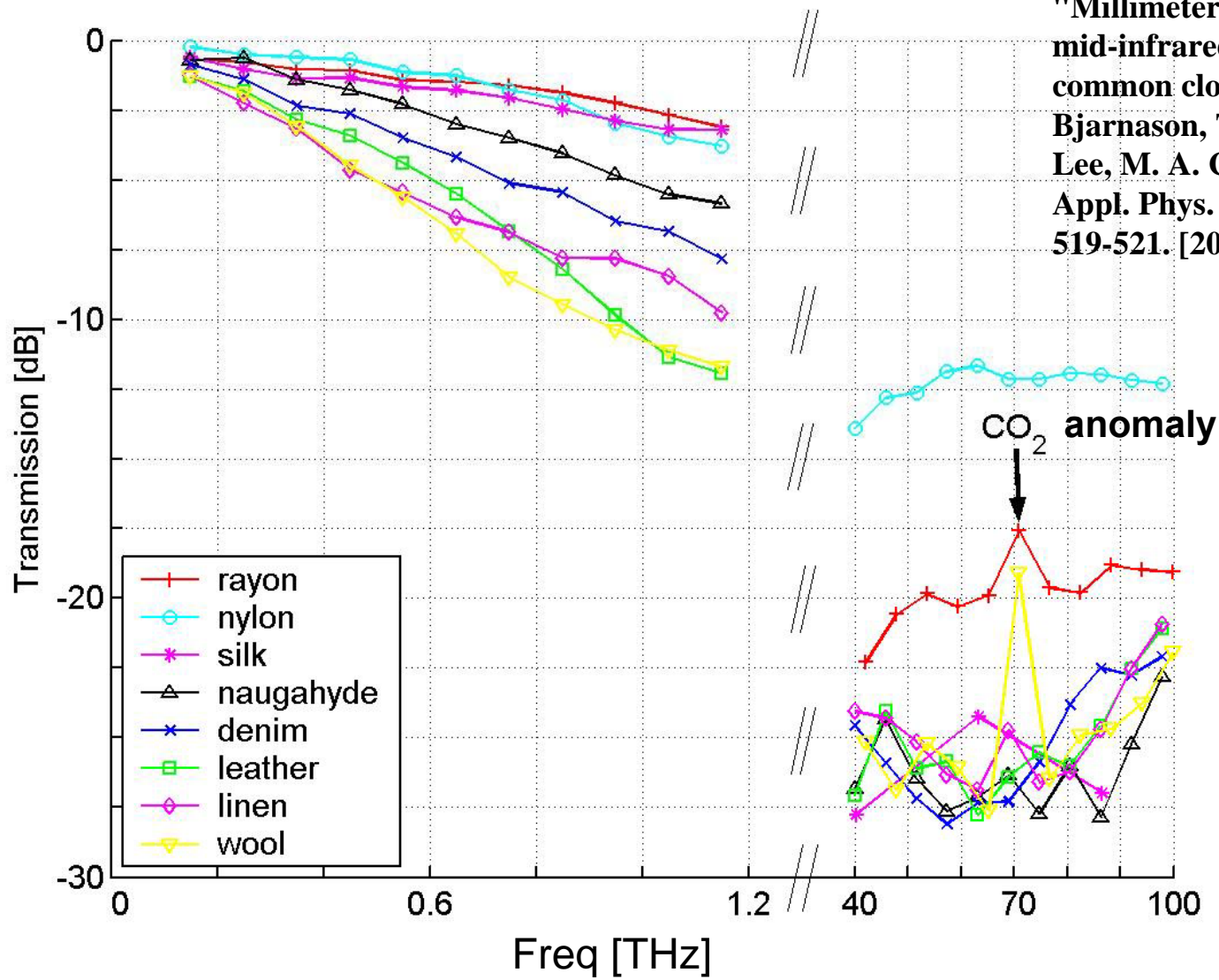
## Common Cloathing Samples
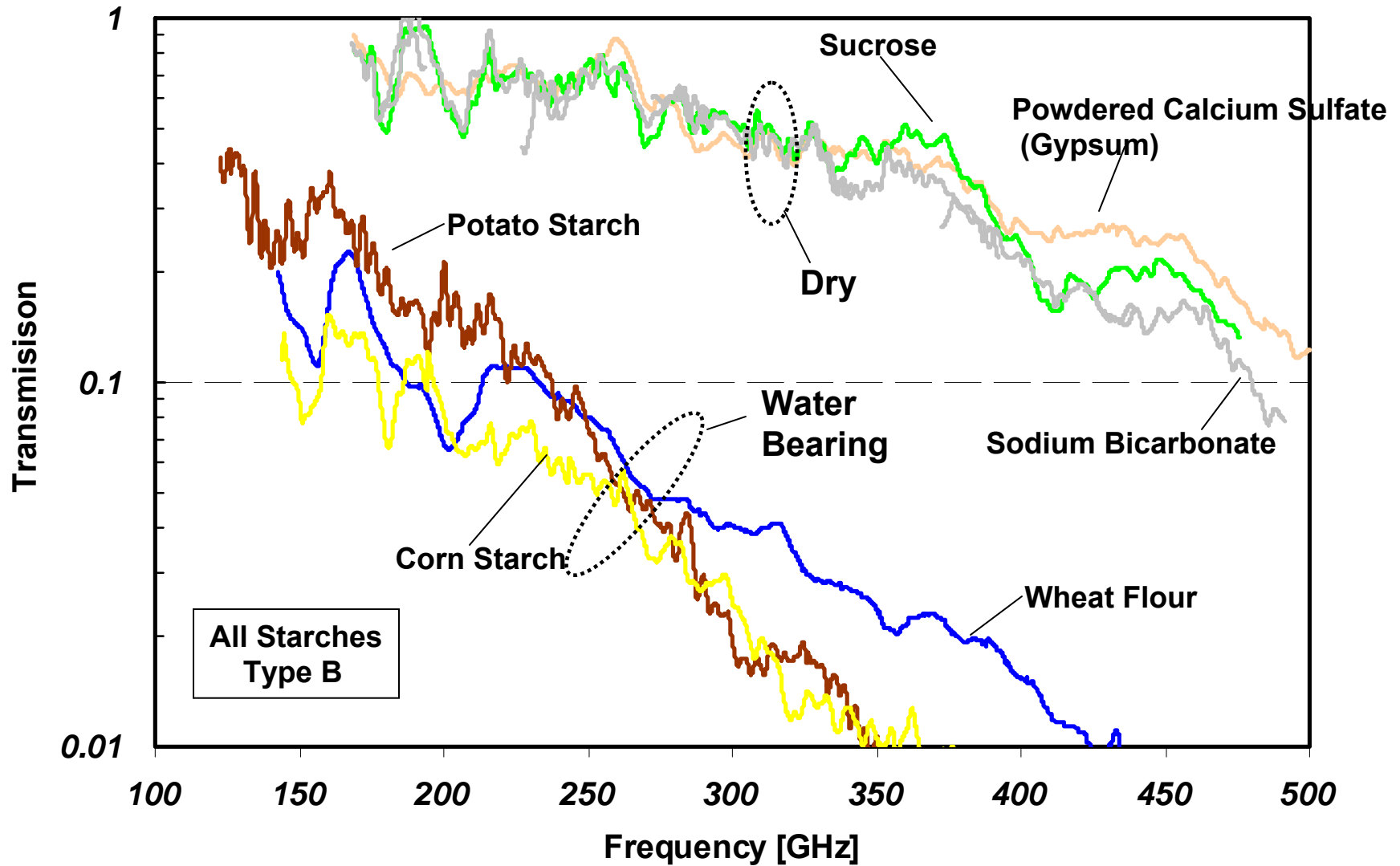
# Transmission through Common Clothing

## (The "Linen Closet")

**"Millimeter-wave, terahertz, and mid-infrared transmission through common clothing" , J. E. Bjarnason, T. L. J. Chan, A. W. M. Lee, M. A. Celis, and E. R. Brown, Appl. Phys. Lett. vol. 85 (no. 4), pp. 519-521. [2004]**
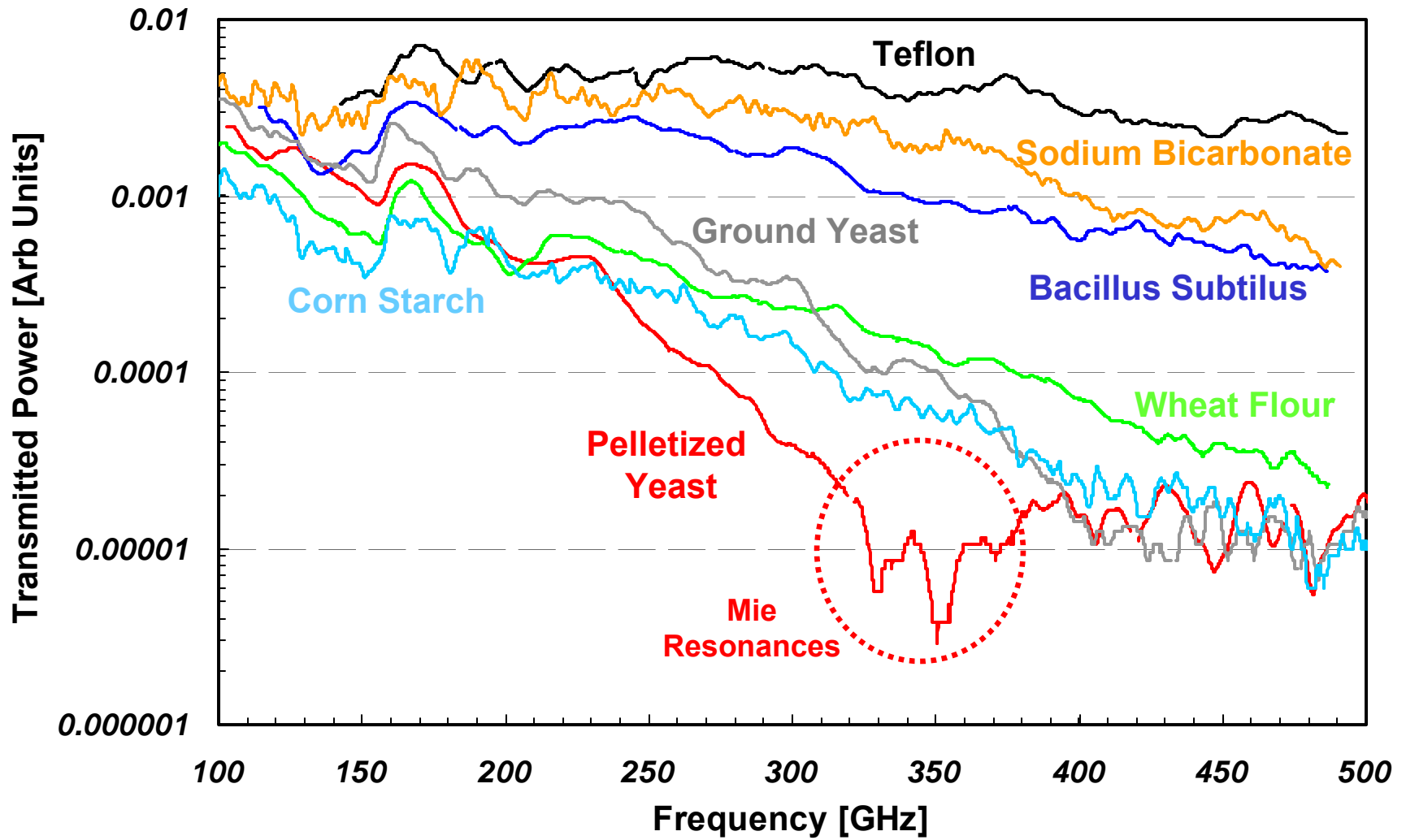
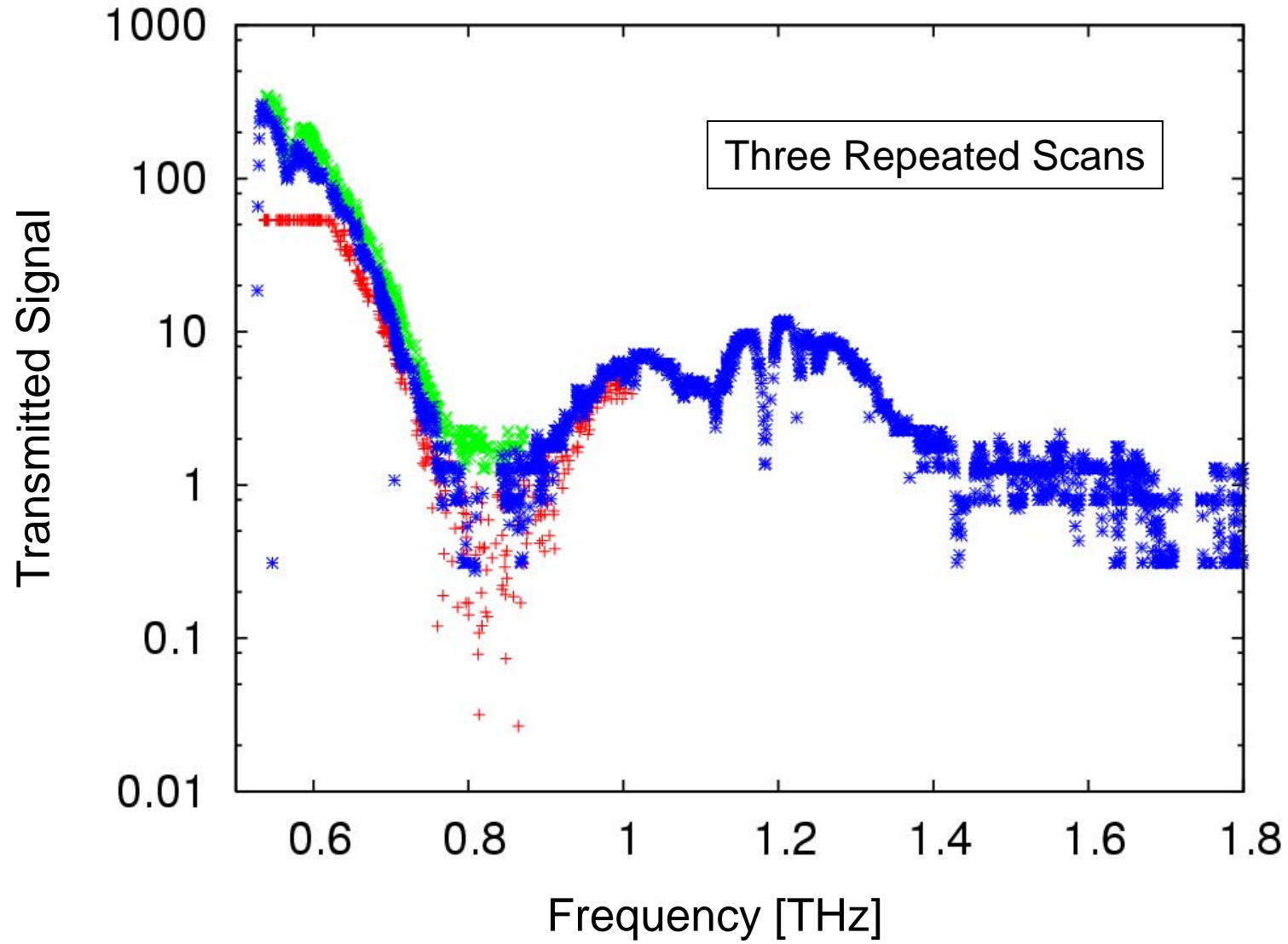# THz Transmission through Organic and Biomaterials
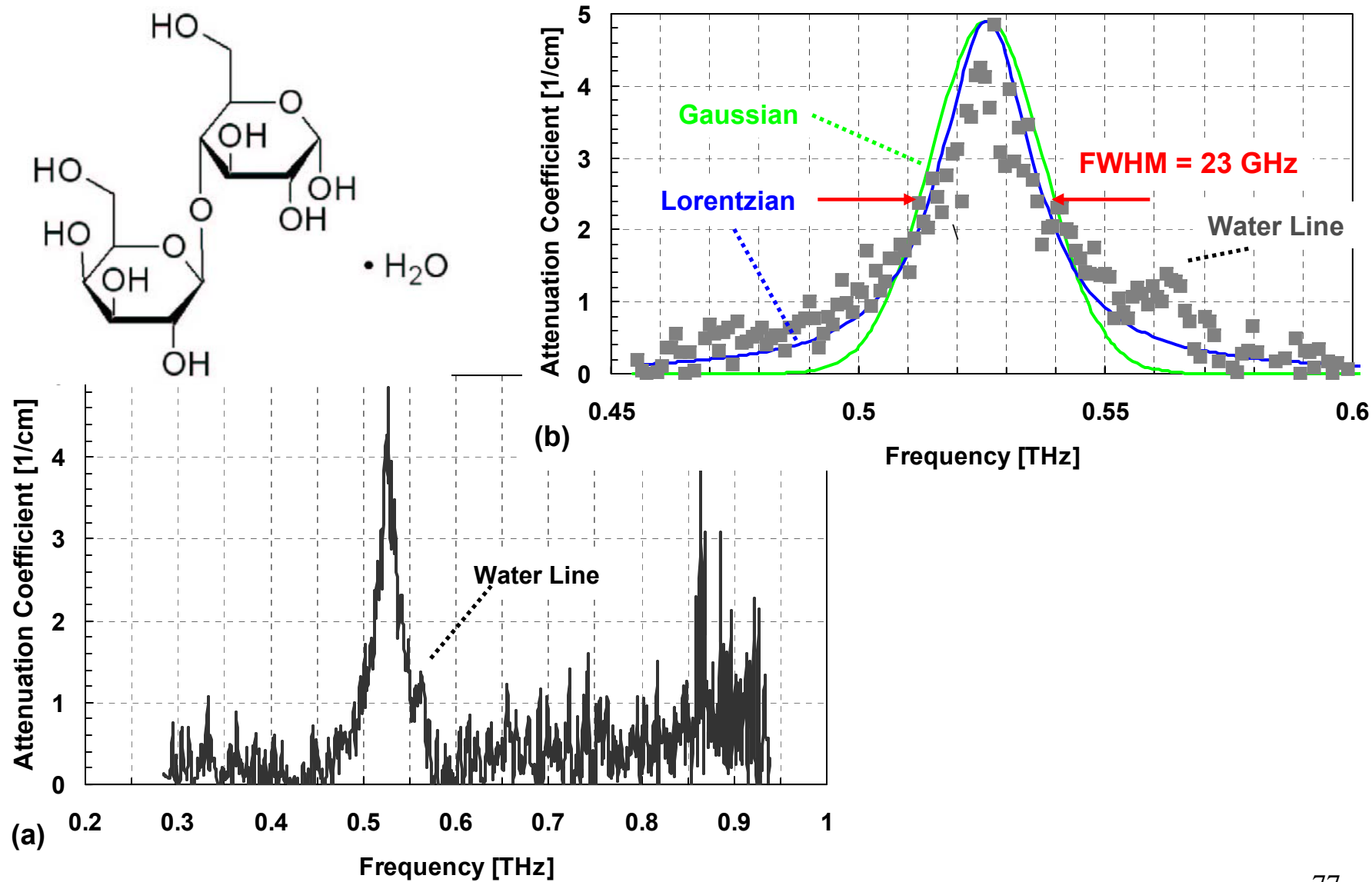
## (The "Kitchen Cupboard")

# THz Transmission through Organic and Biomaterials (cont)

# C4 Explosive (~90% RDX)

# Narrow Macromolecular Resonances
## (Lactose Monohydrate)

# THz Vibrational Resonance of Lactose Monohydrate

**Crystalline**

**Isolated**
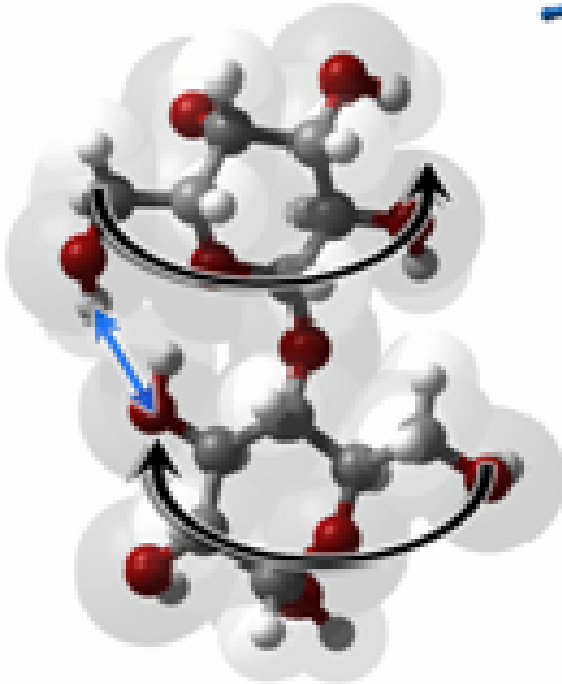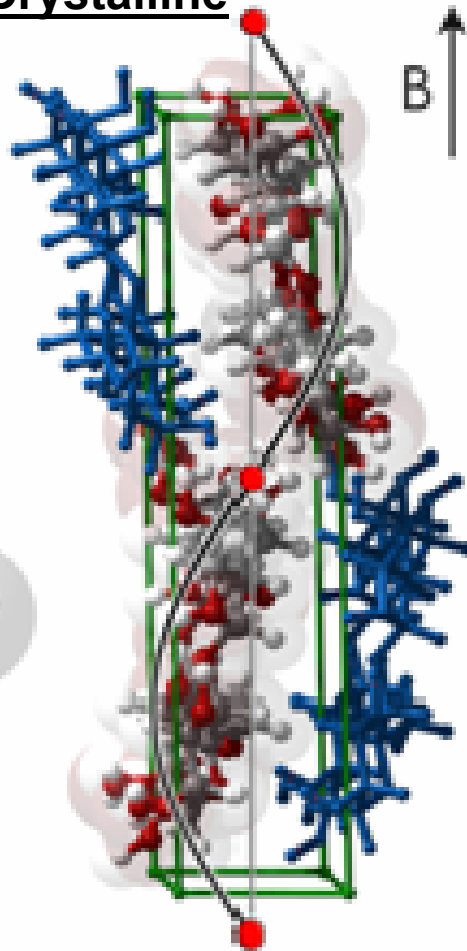


"Assignment of the Lowest-Lying THz Absorption Signatures in Biotin and Lactose Monohydrate by Solid-State Density Functional Theory," D.G. Allis, A.M. Fedor, T.M. Korter , J.E. Bjarnason, and E.R. Brown, accepted to Chem. Phys Lett, Feb. 2007.
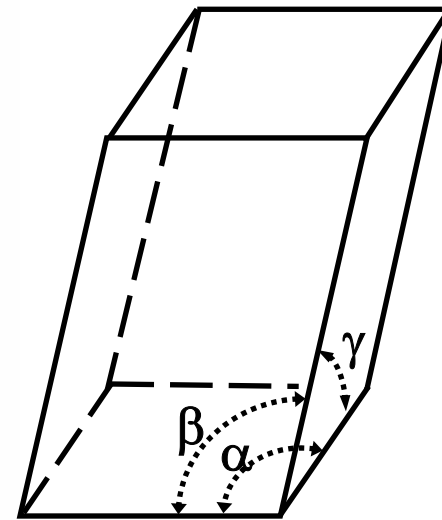
Monoclinic Primitive Unit Cell

**Low-lying Sub-THz resonances can be explained only by combination of intramolecular "twisting" (hindered rotation) plus intermolecular coupling**

## Molecular Absorption Examples (cont)

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• **Recall the change in energy of a rigid diatomic rotor from the state with orbital angular momentum quantum number I to state with I + 1, consistent with absorption of a photon of energy hν:**

$$\Delta U = \frac{\hbar^2}{2I_X}[(l+1)(l+2) - l(l+1)] = \frac{\hbar^2}{I}(l+1) = \hbar\omega \quad \text{or} \quad \nu = \frac{\hbar}{2\pi I}(l+1) \equiv 2B(l+1)$$

**where B is called the rotational constant and I is the moment of inertia.  Recall from mechanics that the moment-of-inertia concept of any three-dimensional solid body of mass M allows us to divide the kinetic energy of the body into two terms: (1) linear KE of the center-of-mass, $(1/2)Mv^2$, and (2) angular kinetic energy of rotation about the center-of-mass point, $(1/2) I\omega^2 = L^2/(2I)$.  It also allows us write**

$$\vec{L} = \overline{\overline{I}}\vec{\omega}$$

**Where ω is a column vector denoting the circular frequency components for an arbitrary rotation about the x, y, and z axes respectively.  This definition reminds us that I is actually a 3x3 matrix, called a** *tensor.  When the rigid body can be approximated as a collection of N masses (very good approximation for any rigid molecule), and in a cartesian coordinate system*

$$\overline{\overline{I}} \equiv \begin{pmatrix} \sum_{i=1}^{N} m_i(y_i^2 + z_i^2) & -\sum_{i=1}^{N} m_i(x_i y_i) & -\sum_{i=1}^{N} m_i(x_i z_i) \\ -\sum_{i=1}^{N} m_i(x_i y_i) & \sum_{i=1}^{N} m_i(x_i^2 + z_i^2) & -\sum_{i=1}^{N} m_i(y_i z_i) \\ -\sum_{i=1}^{N} m_i(x_i z_i) & -\sum_{i=1}^{N} m_i(y_i z_i) & \sum_{i=1}^{N} m_i(x_i^2 + y_i^2) \end{pmatrix}$$

**Note:  this is a real symmetric matrix so from linear algebra can always be diagonalized !**

# Molecular Absorption Examples (cont)

**The diagonal form is defined generically as**

$$\overline{\overline{I}} \equiv \begin{pmatrix} I_X & 0 & 0 \\ 0 & I_Y & 0 \\ 0 & 0 & I_Z \end{pmatrix} \qquad \textbf{satisfying} \qquad \frac{x^2}{I_X} + \frac{y^2}{I_Y} + \frac{z^2}{I_Z} = 1$$

**where $I_X$, $I_Y$, and $I_Z$ are called the "principal" moments of inertia. The right equation is that of an ellipsoid of revolution centered at x=0, y=0, z=0, which is a convenient geometric construct to understand the principal moments.   As in other tensorial quantities in physics, the relative values of $I_X$, $I_Y$, and $I_Z$, reflect the inherent spatial symmetry, so the corresponding objects are given special names**

**(1)     $I_X = I_Y = I_Z$   $\Rightarrow$ spherical "top"**

**(2)     $I_X = I_Y \ne I_Z$   $\Rightarrow$ symmetric "top"**

**(3)     $I_X \ne I_Y \ne I_Z$   $\Rightarrow$ asymmetric "top"**

**(4)     $I_X = I_Y$ ,  $I_Z \approx 0$   $\Rightarrow$ "rotor"**

**(Recall definition of "top": a solid object that can spin freely in any of three dimensions)**

**<u>Rules to determine the principal axes and moments:</u>**
**(1) Any axes of symmetry will generally be a principal axis.**
**        - axis of symmetry means that when rotated about this axis, the molecule reproduces itself every $2\pi/n$ degrees, where n > 2**
**(2)  If a molecule has an axis of symmetry with 3 ≤ n, it will always be a symmetric "top"**

# Molecular Absorption Examples (cont)

**Clearly "rotors" are the simplest since they are effectively one-dimensional**

**(1) Diatomic rotors**



$$I_X = I_Y = \frac{m_1 m_2 R^2}{m_1 + m_2} \rightarrow \mu R^2 \qquad \text{if } m_1 = m_2 \text{, where } \mu \text{ is the "reduced mass"}$$

**(2) Polyatomic (N) rotor**

$$I_X = I_Y = \frac{1}{2} \cdot \frac{\displaystyle\sum_{i=1}^{N}\sum_{j=1}^{N} m_i m_j R_{ij}^2}{\displaystyle\sum_{i=1}^{N} m_i}$$

**(3) Example: Carbon Monoxide:   $m_C$ = 12.0*1.67x10$^{-27}$ KG , $m_O$ = 16.0*1.67x10$^{-27}$ KG, R 1.128 Ang, so that**

**I = 1.457x10$^{-46}$ KG-m$^2$, and $\hbar^2 / I =$ 7.63x10$^{-23}$ J = 0.476 meV or $\nu$ = 115 GHz**

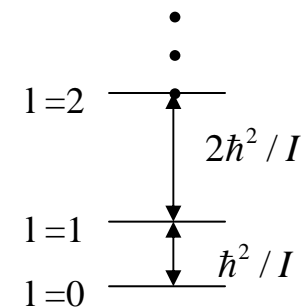**Rotational transition "ladder": $\nu_0$ = 115 GHz $\nu_1$ = 230 GHz $\nu_2$= 345 GHz , etc.**

• **For symmetric rotors (e.g., carbom monoxide CO, hydrogen chloride HCl, etc.), two of the moments (along two orthogonal axes) are identical and the third is trivially small, so that**

$\longleftarrow$ **R** $\longrightarrow$

$(+)$————————$(-)$   $I = \mu R^2$   Ignoring spin, $U_X = \dfrac{L^2}{2I_X}$   $L^2 = \hbar^2 l(l+1)$

$I_X \rightarrow$ **moment of inertia for rotation about a given axis, x**
$L \rightarrow$ **orbital angular momentum eigenvalue**

• **Photon absorption or emission can occur of $\Delta l = 1$, for which**

$l = 2$ —————
$2\hbar^2 / I$
$l = 1$ —————
$\hbar^2 / I$
$l = 0$ —————

**This creates a "ladder" of photon frequencies as shown to the right**

• **Although highly polar, water is asymmetric rotor meaning that no two moments of inertia are equal. This follows from its non-colinear alignment between the three atoms**

$104.45°$

$0.9584$ Å

• **Any of these purely rotational transitions will be easily observed if $\omega\tau \gg 1$   where $\tau$ is the momentum relaxation time (or dephasing time)**

• **Generally, $\tau > 100$ ps or more under STP conditions, so THz transitions are obvious**

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